Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:23 am BST

PDB ID	:	4GCT
Title	:	structure of No factor protein-DNA complex
Authors	:	Schumacher, M.A.
Deposited on	:	2012-07-30
Resolution	:	2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

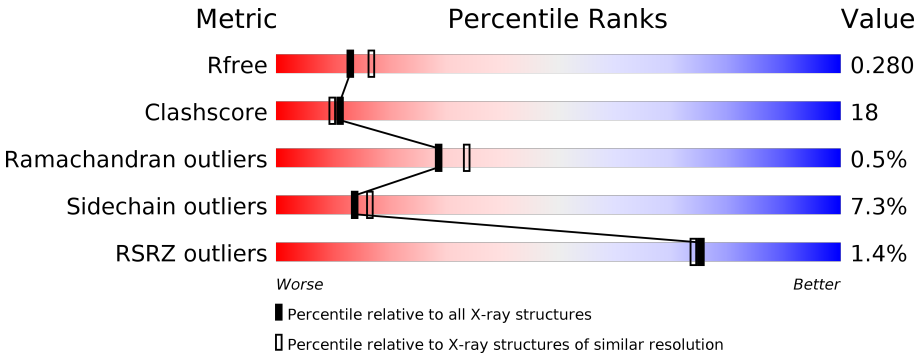
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	196	2% 65% 26% 6%
1	B	196	2% 62% 32%
1	C	196	2% 62% 31%
1	D	196	2% 56% 37%
2	W	20	5% 40% 60%
2	Z	20	40% 55% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7196 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nucleoid occlusion factor SlmA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1505	950	271	279	5			
1	B	189	Total	C	N	O	S	0	0	0
			1543	973	283	282	5			
1	C	190	Total	C	N	O	S	0	0	0
			1559	983	284	287	5			
1	D	189	Total	C	N	O	S	0	0	0
			1547	975	283	284	5			

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*TP*AP*CP*GP*TP*GP*AP*GP*TP*AP*CP*TP*CP*AP*CP*GP*TP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	20	Total	C	N	O	P	0	0	0
			407	196	74	118	19			
2	Z	20	Total	C	N	O	P	0	0	0
			407	196	74	118	19			

- Molecule 3 is water.

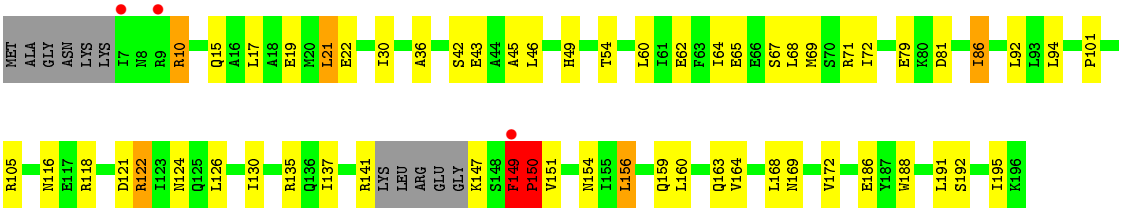
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	52	Total	O	0	0
			52	52		
3	B	51	Total	O	0	0
			51	51		
3	C	52	Total	O	0	0
			52	52		
3	D	46	Total	O	0	0
			46	46		
3	W	16	Total	O	0	0
			16	16		
3	Z	11	Total	O	0	0
			11	11		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

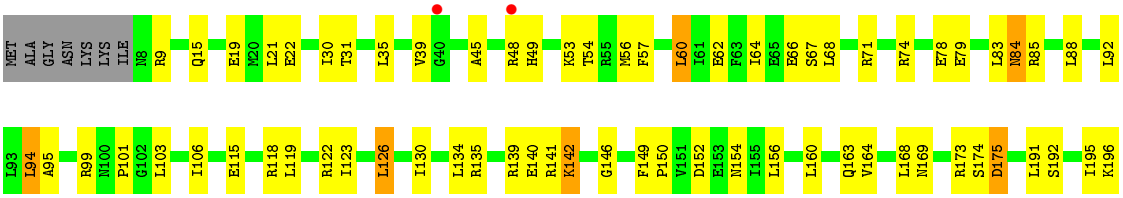
- Molecule 1: Nucleoid occlusion factor SlmA

Chain A:



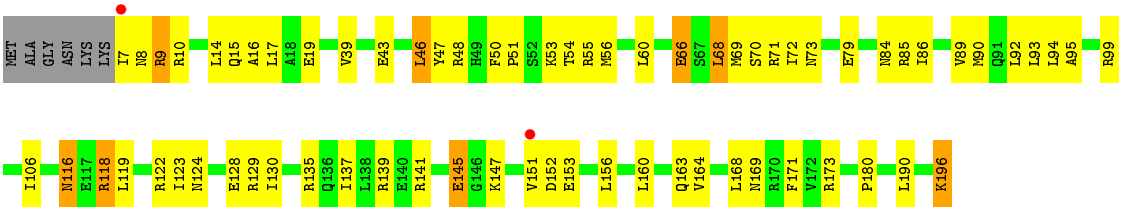
- Molecule 1: Nucleoid occlusion factor SlmA

Chain B:



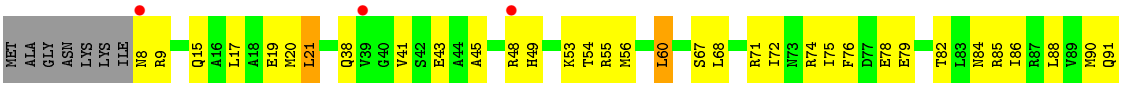
- Molecule 1: Nucleoid occlusion factor SlmA

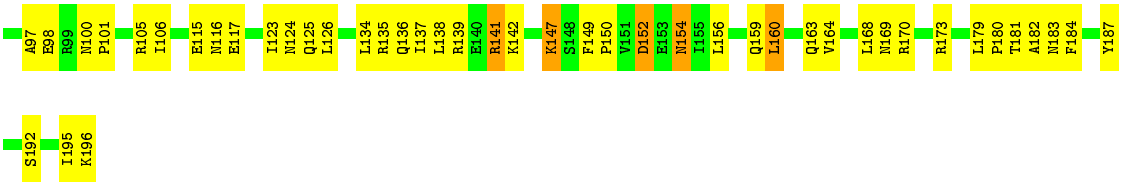
Chain C:



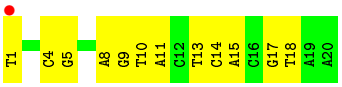
- Molecule 1: Nucleoid occlusion factor SlmA

Chain D:





• Molecule 2: DNA (5'-D(*TP*TP*AP*CP*GP*TP*GP*AP*GP*TP*AP*CP*TP*CP*AP*CP *GP*TP*AP*A)-3')



• Molecule 2: DNA (5'-D(*TP*TP*AP*CP*GP*TP*GP*AP*GP*TP*AP*CP*TP*CP*AP*CP *GP*TP*AP*A)-3')

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.10Å 61.36Å 121.08Å 90.00° 99.06° 90.00°	Depositor
Resolution (Å)	63.75 – 2.45 63.74 – 2.45	Depositor EDS
% Data completeness (in resolution range)	90.7 (63.75-2.45) 90.8 (63.74-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.45Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.225 , 0.276 0.231 , 0.280	Depositor DCC
R_{free} test set	2678 reflections (7.91%)	wwPDB-VP
Wilson B-factor (Å^2)	48.9	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 39.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7196	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2254e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.51	3/1525 (0.2%)	0.66	4/2046 (0.2%)
1	B	0.40	0/1564	0.57	0/2097
1	C	0.40	0/1580	0.54	0/2118
1	D	0.41	0/1568	0.57	0/2102
2	W	0.35	0/456	0.69	0/702
2	Z	0.62	1/456 (0.2%)	0.85	2/702 (0.3%)
All	All	0.44	4/7149 (0.1%)	0.61	6/9767 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	Z	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	PHE	CA-C	6.71	1.70	1.52
1	A	149	PHE	C-N	6.53	1.46	1.34
1	A	149	PHE	N-CA	6.00	1.58	1.46
2	Z	19	DT	C1'-N1	5.34	1.56	1.49

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	150	PRO	CA-N-CD	-9.90	97.63	111.50
2	Z	19	DT	O4'-C1'-N1	9.32	114.53	108.00
1	A	149	PHE	CB-CA-C	6.68	123.77	110.40
1	A	149	PHE	N-CA-CB	-5.81	100.14	110.60
2	Z	19	DT	C6-N1-C2	-5.67	118.47	121.30
1	A	150	PRO	N-CA-CB	5.18	109.52	103.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Z	19	DT	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1505	0	1518	44	0
1	B	1543	0	1573	60	0
1	C	1559	0	1592	68	0
1	D	1547	0	1577	62	0
2	W	407	0	228	15	0
2	Z	407	0	228	15	0
3	A	52	0	0	1	0
3	B	51	0	0	3	0
3	C	52	0	0	0	0
3	D	46	0	0	0	0
3	W	16	0	0	1	0
3	Z	11	0	0	0	0
All	All	7196	0	6716	244	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (244) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:8:DA:H1'	2:W:9:DG:H5'	1.52	0.89
1:B:62:GLU:HG3	1:B:122:ARG:HH22	1.37	0.88
1:D:48:ARG:HH12	2:W:1:DT:H5'	1.34	0.88
2:W:4:DC:H1'	2:W:5:DG:H5'	1.56	0.87
1:B:54:THR:HG21	1:B:118:ARG:HD3	1.57	0.85
1:B:141:ARG:HH22	1:B:196:LYS:HA	1.41	0.85
1:B:15:GLN:O	1:B:19:GLU:HG3	1.78	0.83
1:C:79:GLU:O	1:C:85:ARG:HD3	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:ARG:NH1	2:W:1:DT:H5'	1.95	0.81
1:C:163:GLN:NE2	1:D:159:GLN:HG3	2.00	0.77
1:B:83:LEU:HD11	1:B:196:LYS:HG2	1.68	0.76
1:B:62:GLU:HG3	1:B:122:ARG:NH2	2.01	0.76
2:Z:20:DT:H2"	2:Z:21:DA:H5'	1.69	0.75
1:C:118:ARG:HH11	1:C:119:LEU:HD23	1.51	0.74
1:D:82:THR:HG21	1:D:141:ARG:HG3	1.70	0.74
1:C:54:THR:HG21	1:C:116:ASN:ND2	2.03	0.73
1:C:135:ARG:HH12	1:C:153:GLU:HB2	1.55	0.72
1:D:68:LEU:O	1:D:72:ILE:HG12	1.89	0.72
1:B:79:GLU:O	1:B:85:ARG:HD2	1.91	0.70
1:D:139:ARG:HG3	1:D:139:ARG:HH11	1.56	0.69
1:C:116:ASN:HB2	1:C:118:ARG:HG3	1.75	0.69
1:A:169:ASN:HD21	1:B:169:ASN:ND2	1.91	0.69
1:B:9:ARG:HG2	1:B:49:HIS:CE1	2.27	0.68
1:B:141:ARG:NH2	1:B:196:LYS:HA	2.09	0.68
1:C:86:ILE:HG13	1:C:137:ILE:HG21	1.77	0.67
1:B:48:ARG:HH22	2:Z:19:DT:H2'	1.60	0.67
2:Z:22:DC:H2"	2:Z:23:DG:O5'	1.94	0.67
1:A:69:MET:CE	1:A:130:ILE:HD13	2.25	0.66
1:A:163:GLN:NE2	1:B:163:GLN:HG2	2.11	0.66
1:B:48:ARG:NH2	2:Z:19:DT:H2'	2.10	0.66
1:A:149:PHE:O	1:A:151:VAL:HG23	1.96	0.65
1:B:53:LYS:HA	1:B:56:MET:CE	2.26	0.65
1:D:182:ALA:O	1:D:183:ASN:HB2	1.97	0.65
1:C:85:ARG:O	1:C:89:VAL:HG23	1.96	0.65
1:D:15:GLN:O	1:D:19:GLU:HG3	1.97	0.65
1:D:54:THR:HG21	1:D:116:ASN:HB2	1.79	0.65
1:C:106:ILE:HG22	1:C:123:ILE:HD11	1.79	0.64
2:Z:28:DT:H2"	2:Z:29:DA:C8	2.33	0.64
1:D:156:LEU:HD11	1:D:195:ILE:HD12	1.78	0.64
1:D:192:SER:O	1:D:196:LYS:HB2	1.98	0.64
1:A:169:ASN:ND2	1:B:169:ASN:ND2	2.46	0.63
1:C:141:ARG:HG2	1:C:147:LYS:HG3	1.77	0.63
1:C:90:MET:CE	1:C:160:LEU:HB3	2.27	0.63
1:C:124:ASN:O	1:C:128:GLU:HG2	2.00	0.62
1:D:20:MET:SD	1:D:38:GLN:HG3	2.40	0.62
1:A:22:GLU:HG3	1:A:101:PRO:HB2	1.81	0.61
1:B:169:ASN:O	1:B:173:ARG:HB2	2.01	0.60
1:D:135:ARG:HD3	1:D:154:ASN:ND2	2.17	0.60
1:C:145:GLU:O	1:C:147:LYS:HE3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ARG:HD2	1:A:92:LEU:HD11	1.83	0.60
1:D:17:LEU:O	1:D:21:LEU:HD22	2.02	0.59
1:A:54:THR:HG21	1:A:116:ASN:HB2	1.85	0.58
1:C:90:MET:HE3	1:C:160:LEU:HB3	1.85	0.58
1:C:71:ARG:HD2	1:C:92:LEU:HD21	1.85	0.58
3:B:218:HOH:O	2:W:15:DA:H5"	2.03	0.58
2:Z:24:DT:H2"	2:Z:25:DG:N7	2.18	0.58
1:B:53:LYS:HA	1:B:56:MET:HE3	1.85	0.58
1:A:121:ASP:HB2	3:A:238:HOH:O	2.03	0.58
1:A:156:LEU:CD2	1:A:160:LEU:HD13	2.34	0.58
1:A:126:LEU:O	1:A:130:ILE:HG12	2.04	0.57
1:B:21:LEU:HD13	1:B:30:ILE:CD1	2.34	0.57
1:D:91:GLN:HB2	1:D:184:PHE:CZ	2.41	0.56
1:C:151:VAL:HG22	1:C:152:ASP:N	2.21	0.56
1:D:139:ARG:NH1	1:D:139:ARG:HG3	2.20	0.56
1:B:141:ARG:HD2	1:B:149:PHE:CZ	2.41	0.55
1:D:9:ARG:HH11	1:D:41:VAL:HG11	1.71	0.55
1:C:118:ARG:HH11	1:C:119:LEU:CD2	2.19	0.55
1:D:79:GLU:HG2	1:D:84:ASN:HB3	1.88	0.55
1:D:139:ARG:NH2	1:D:154:ASN:HD21	2.04	0.54
1:C:151:VAL:HG22	1:C:152:ASP:H	1.71	0.54
1:C:71:ARG:CZ	1:C:99:ARG:NH2	2.71	0.54
1:B:74:ARG:HG2	1:B:78:GLU:OE2	2.07	0.54
1:C:51:PRO:HG2	1:C:55:ARG:HG3	1.89	0.53
1:A:149:PHE:O	1:A:150:PRO:C	2.46	0.53
1:B:149:PHE:HB3	1:B:150:PRO:HD2	1.91	0.53
1:A:69:MET:HE3	1:A:130:ILE:HD13	1.89	0.53
1:C:90:MET:O	1:C:94:LEU:HD13	2.09	0.53
1:D:142:LYS:HA	1:D:147:LYS:O	2.08	0.53
1:B:71:ARG:HH11	1:B:92:LEU:HD11	1.73	0.53
1:A:10:ARG:HG3	1:A:49:HIS:HB3	1.90	0.53
1:B:135:ARG:O	1:B:139:ARG:HG3	2.08	0.53
1:D:9:ARG:HH21	1:D:9:ARG:HG2	1.74	0.53
2:W:17:DG:H2'	2:W:18:DT:C6	2.44	0.52
1:A:65:GLU:HG2	1:A:126:LEU:HD13	1.92	0.52
1:C:69:MET:HE1	1:C:72:ILE:HD12	1.90	0.52
1:D:139:ARG:HH21	1:D:154:ASN:HD21	1.58	0.52
2:W:8:DA:C1'	2:W:9:DG:H5'	2.34	0.52
1:A:156:LEU:HD22	1:A:160:LEU:HD13	1.92	0.52
1:B:71:ARG:HH11	1:B:71:ARG:HG3	1.74	0.52
1:C:169:ASN:HD21	1:D:169:ASN:CG	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ASN:O	1:B:88:LEU:HG	2.10	0.52
1:A:94:LEU:CD1	1:A:164:VAL:HG13	2.40	0.52
1:B:67:SER:O	1:B:71:ARG:HG3	2.09	0.52
1:C:141:ARG:O	1:C:145:GLU:HG3	2.09	0.51
1:D:71:ARG:HH11	1:D:71:ARG:HG2	1.76	0.51
1:C:106:ILE:CG2	1:C:123:ILE:HD11	2.39	0.51
1:C:135:ARG:HH11	1:C:135:ARG:HG2	1.76	0.51
1:C:7:ILE:HG22	1:C:8:ASN:N	2.26	0.51
1:A:192:SER:HA	1:A:195:ILE:HG22	1.93	0.51
1:B:57:PHE:CD2	1:B:115:GLU:HG2	2.46	0.51
1:C:90:MET:HE1	1:C:160:LEU:HB3	1.92	0.51
2:W:4:DC:H1'	2:W:5:DG:C5'	2.37	0.51
1:A:135:ARG:HD3	1:A:154:ASN:HA	1.93	0.50
2:Z:19:DT:H2"	2:Z:20:DT:OP2	2.10	0.50
1:A:65:GLU:OE2	1:A:122:ARG:NH1	2.44	0.50
1:C:7:ILE:HB	1:C:10:ARG:HB3	1.93	0.50
2:W:10:DT:H5'	3:W:102:HOH:O	2.11	0.50
1:C:106:ILE:HG22	1:C:123:ILE:CD1	2.41	0.50
1:A:54:THR:CG2	1:A:116:ASN:HB2	2.41	0.50
1:A:69:MET:CE	1:A:72:ILE:HD12	2.42	0.50
1:C:141:ARG:HA	1:C:145:GLU:HG3	1.93	0.49
1:C:15:GLN:O	1:C:19:GLU:HG3	2.12	0.49
1:A:67:SER:O	1:A:71:ARG:HG3	2.12	0.49
1:A:69:MET:HE1	1:A:130:ILE:HD13	1.94	0.49
1:D:170:ARG:HG2	1:D:173:ARG:HH21	1.76	0.49
1:A:79:GLU:OE1	1:A:81:ASP:HB3	2.13	0.49
1:B:21:LEU:HD13	1:B:30:ILE:HD11	1.93	0.49
1:B:71:ARG:HG3	1:B:71:ARG:NH1	2.28	0.49
1:A:65:GLU:CG	1:A:126:LEU:HD13	2.42	0.49
1:C:190:LEU:HD23	1:C:190:LEU:O	2.13	0.49
1:B:54:THR:HG22	1:B:118:ARG:NH1	2.27	0.48
1:C:95:ALA:O	1:C:99:ARG:HG2	2.13	0.48
1:A:118:ARG:O	1:A:121:ASP:HB3	2.12	0.48
1:D:76:PHE:CZ	1:D:137:ILE:HG13	2.49	0.48
1:D:9:ARG:NH2	1:D:9:ARG:HG2	2.29	0.48
1:A:124:ASN:OD1	1:B:173:ARG:HD2	2.14	0.48
1:A:21:LEU:HD13	1:A:30:ILE:CD1	2.44	0.47
1:D:45:ALA:HA	1:D:48:ARG:HD2	1.97	0.47
1:A:36:ALA:HA	1:A:46:LEU:HD21	1.96	0.47
1:C:66:GLU:HA	1:C:66:GLU:OE1	2.13	0.47
1:C:93:LEU:HD21	1:C:130:ILE:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:SER:O	1:D:71:ARG:HG3	2.14	0.47
1:B:142:LYS:O	1:B:146:GLY:HA2	2.15	0.47
1:B:53:LYS:HA	1:B:56:MET:HE2	1.95	0.47
2:Z:23:DG:H2'	2:Z:24:DT:C7	2.45	0.47
1:B:54:THR:CG2	1:B:118:ARG:HH11	2.28	0.47
1:B:115:GLU:HB3	1:B:119:LEU:HD12	1.97	0.47
1:D:54:THR:CG2	1:D:116:ASN:HB2	2.44	0.47
1:B:94:LEU:CD1	1:B:164:VAL:HG22	2.45	0.47
1:C:164:VAL:O	1:C:168:LEU:HG	2.15	0.47
1:D:48:ARG:HG3	1:D:49:HIS:CE1	2.49	0.47
1:A:62:GLU:CG	1:A:122:ARG:HH22	2.28	0.47
1:B:9:ARG:HG2	1:B:49:HIS:NE2	2.29	0.47
1:D:179:LEU:HA	1:D:180:PRO:HD3	1.79	0.47
1:D:86:ILE:O	1:D:90:MET:HG2	2.16	0.46
1:C:69:MET:SD	1:C:129:ARG:NH1	2.89	0.46
1:B:141:ARG:HH22	1:B:196:LYS:CA	2.18	0.46
1:C:43:GLU:O	1:C:46:LEU:HB2	2.16	0.46
1:D:75:ILE:HD13	1:D:88:LEU:HB3	1.98	0.46
1:C:93:LEU:HD11	1:C:130:ILE:HD13	1.97	0.46
1:D:149:PHE:HB3	1:D:150:PRO:HD2	1.98	0.46
1:D:156:LEU:CD2	1:D:160:LEU:HD22	2.45	0.46
1:A:141:ARG:O	1:A:147:LYS:HA	2.16	0.46
1:B:35:LEU:O	1:B:39:VAL:HG23	2.16	0.46
1:C:118:ARG:HD3	1:C:119:LEU:HD23	1.98	0.45
1:C:7:ILE:HG22	1:C:8:ASN:H	1.79	0.45
1:A:86:ILE:HG12	1:A:137:ILE:HG21	1.97	0.45
1:D:91:GLN:HB2	1:D:184:PHE:CE2	2.51	0.45
1:B:45:ALA:HA	1:B:48:ARG:NH1	2.31	0.45
1:B:169:ASN:HB2	3:B:227:HOH:O	2.15	0.45
1:B:64:ILE:HD11	1:B:103:LEU:HB3	1.99	0.45
1:D:152:ASP:OD1	1:D:154:ASN:N	2.49	0.45
1:B:31:THR:HG22	2:W:14:DC:H3'	1.97	0.45
1:D:60:LEU:HD23	1:D:106:ILE:HD11	1.99	0.45
1:D:60:LEU:HD23	1:D:106:ILE:CD1	2.47	0.44
1:D:48:ARG:NH1	2:W:1:DT:H6	2.16	0.44
2:Z:23:DG:H2'	2:Z:24:DT:C6	2.51	0.44
1:B:164:VAL:O	1:B:168:LEU:HG	2.17	0.44
1:A:168:LEU:O	1:A:172:VAL:HG23	2.17	0.44
1:A:60:LEU:O	1:A:64:ILE:HG13	2.18	0.44
1:C:190:LEU:HD23	1:C:190:LEU:C	2.38	0.44
1:D:45:ALA:O	1:D:48:ARG:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ALA:CB	1:C:39:VAL:HG22	2.48	0.44
1:C:53:LYS:HE3	2:W:11:DA:OP1	2.17	0.44
1:C:47:TYR:HA	1:C:50:PHE:O	2.18	0.44
1:C:10:ARG:HG2	1:C:10:ARG:HH11	1.82	0.44
1:C:51:PRO:CG	1:C:55:ARG:HG3	2.48	0.44
1:A:21:LEU:HA	1:A:21:LEU:HD12	1.86	0.43
1:B:126:LEU:O	1:B:130:ILE:HG13	2.18	0.43
1:B:54:THR:HG23	1:B:119:LEU:HD11	1.99	0.43
1:B:94:LEU:HD11	1:B:164:VAL:HG22	2.00	0.43
1:D:100:ASN:N	1:D:101:PRO:HD3	2.33	0.43
1:D:164:VAL:O	1:D:168:LEU:HG	2.18	0.43
1:B:85:ARG:NH2	1:B:140:GLU:OE2	2.51	0.43
1:D:156:LEU:HD23	1:D:156:LEU:O	2.18	0.43
2:W:13:DT:C2	2:Z:27:DG:N2	2.85	0.43
1:D:123:ILE:HA	1:D:123:ILE:HD13	1.93	0.43
1:D:86:ILE:HD11	1:D:138:LEU:HD23	2.00	0.43
1:C:163:GLN:HE21	1:D:159:GLN:HG3	1.79	0.43
1:D:21:LEU:O	1:D:105:ARG:HD2	2.19	0.43
1:C:71:ARG:NH2	1:C:99:ARG:NH2	2.66	0.43
2:Z:23:DG:H2'	2:Z:24:DT:H72	1.99	0.43
1:A:42:SER:O	1:A:45:ALA:HB3	2.19	0.43
1:A:69:MET:HE2	1:A:72:ILE:HD12	1.99	0.43
1:D:163:GLN:NE2	1:D:187:TYR:OH	2.50	0.43
1:C:156:LEU:O	1:C:160:LEU:HG	2.19	0.43
2:Z:27:DG:C2'	2:Z:28:DT:H5"	2.49	0.43
1:C:116:ASN:N	1:C:116:ASN:OD1	2.52	0.42
1:B:66:GLU:CB	3:B:225:HOH:O	2.67	0.42
1:C:196:LYS:HE2	1:C:196:LYS:O	2.19	0.42
1:D:154:ASN:N	1:D:154:ASN:HD22	2.17	0.42
1:B:123:ILE:HA	1:B:123:ILE:HD13	1.87	0.42
1:B:196:LYS:HB3	1:B:196:LYS:HE2	1.94	0.42
1:C:119:LEU:O	1:C:122:ARG:HB2	2.20	0.42
1:B:60:LEU:HD12	1:B:60:LEU:HA	1.82	0.42
2:Z:21:DA:H2"	2:Z:22:DC:O5'	2.19	0.42
1:A:17:LEU:O	1:A:21:LEU:HB2	2.20	0.42
1:C:53:LYS:O	1:C:56:MET:HB2	2.19	0.42
1:C:152:ASP:OD1	1:C:153:GLU:N	2.53	0.42
1:B:95:ALA:O	1:B:99:ARG:HG3	2.20	0.42
1:D:170:ARG:HG2	1:D:173:ARG:NH2	2.34	0.42
1:D:74:ARG:O	1:D:78:GLU:HG3	2.19	0.42
1:B:152:ASP:OD1	1:B:154:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:LEU:HD22	1:C:60:LEU:CD1	2.50	0.41
1:B:192:SER:O	1:B:196:LYS:HG3	2.21	0.41
1:B:21:LEU:HD13	1:B:30:ILE:HD12	2.01	0.41
1:D:55:ARG:HA	1:D:55:ARG:HD3	1.92	0.41
1:A:86:ILE:HG22	1:A:188:TRP:CZ3	2.55	0.41
1:D:97:ALA:CB	1:D:168:LEU:HD22	2.51	0.41
1:D:79:GLU:O	1:D:85:ARG:HD2	2.19	0.41
1:C:68:LEU:O	1:C:72:ILE:HG13	2.20	0.41
1:C:171:PHE:CD1	1:C:180:PRO:HD3	2.55	0.41
1:B:173:ARG:C	1:B:175:ASP:H	2.24	0.41
1:C:163:GLN:OE1	1:C:163:GLN:HA	2.21	0.41
1:C:9:ARG:HG3	2:Z:23:DG:OP2	2.21	0.41
1:D:48:ARG:NH2	2:W:1:DT:H73	2.35	0.41
1:B:142:LYS:HG2	1:B:142:LYS:H	1.52	0.41
1:C:10:ARG:NH1	1:C:10:ARG:HG2	2.35	0.41
1:D:53:LYS:O	1:D:56:MET:HB2	2.20	0.41
2:Z:37:DA:H2"	2:Z:38:DA:OP2	2.21	0.41
1:A:94:LEU:CD1	1:A:164:VAL:HG22	2.51	0.41
1:C:139:ARG:HG3	1:C:139:ARG:HH11	1.86	0.41
1:D:48:ARG:HH12	2:W:1:DT:H6	1.69	0.41
1:D:98:GLU:OE1	1:D:181:THR:OG1	2.38	0.41
1:A:186:GLU:N	1:A:186:GLU:OE1	2.54	0.41
1:B:22:GLU:HG3	1:B:101:PRO:HB2	2.02	0.40
1:C:14:LEU:HD22	1:C:60:LEU:HD13	2.03	0.40
1:A:43:GLU:HA	1:A:46:LEU:HD23	2.04	0.40
1:C:39:VAL:O	1:C:39:VAL:HG12	2.22	0.40
1:B:103:LEU:O	1:B:106:ILE:HB	2.21	0.40
1:C:173:ARG:HB3	1:D:124:ASN:OD1	2.21	0.40
1:C:73:ASN:HA	1:C:73:ASN:HD22	1.70	0.40
1:C:163:GLN:HE22	1:D:159:GLN:HG3	1.83	0.40
1:A:68:LEU:O	1:A:72:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	181/196 (92%)	174 (96%)	5 (3%)	2 (1%)	14 14
1	B	187/196 (95%)	177 (95%)	8 (4%)	2 (1%)	14 14
1	C	188/196 (96%)	178 (95%)	10 (5%)	0	100 100
1	D	187/196 (95%)	179 (96%)	8 (4%)	0	100 100
All	All	743/784 (95%)	708 (95%)	31 (4%)	4 (0%)	29 34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	PRO
1	B	195	ILE
1	B	174	SER
1	A	149	PHE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	160/171 (94%)	150 (94%)	10 (6%)	18 22
1	B	164/171 (96%)	153 (93%)	11 (7%)	16 20
1	C	167/171 (98%)	155 (93%)	12 (7%)	14 17
1	D	165/171 (96%)	150 (91%)	15 (9%)	9 10
All	All	656/684 (96%)	608 (93%)	48 (7%)	14 16

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	15	GLN
1	A	19	GLU
1	A	21	LEU

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Mol	Chain	Res	Type
1	A	86	ILE
1	A	105	ARG
1	A	122	ARG
1	A	156	LEU
1	A	159	GLN
1	A	191	LEU
1	B	60	LEU
1	B	68	LEU
1	B	84	ASN
1	B	94	LEU
1	B	126	LEU
1	B	134	LEU
1	B	142	LYS
1	B	156	LEU
1	B	160	LEU
1	B	175	ASP
1	B	191	LEU
1	C	9	ARG
1	C	17	LEU
1	C	46	LEU
1	C	48	ARG
1	C	66	GLU
1	C	68	LEU
1	C	70	SER
1	C	84	ASN
1	C	116	ASN
1	C	118	ARG
1	C	145	GLU
1	C	196	LYS
1	D	8	ASN
1	D	21	LEU
1	D	43	GLU
1	D	60	LEU
1	D	115	GLU
1	D	117	GLU
1	D	125	GLN
1	D	126	LEU
1	D	134	LEU
1	D	136	GLN
1	D	141	ARG
1	D	147	LYS
1	D	152	ASP

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Mol	Chain	Res	Type
1	D	154	ASN
1	D	160	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	73	ASN
1	A	125	GLN
1	A	136	GLN
1	A	159	GLN
1	A	163	GLN
1	B	154	ASN
1	B	169	ASN
1	B	194	GLN
1	C	15	GLN
1	C	73	ASN
1	C	91	GLN
1	C	159	GLN
1	C	169	ASN
1	D	8	ASN
1	D	15	GLN
1	D	154	ASN
1	D	159	GLN
1	D	163	GLN
1	D	169	ASN
1	D	194	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	185/196 (94%)	0.04	3 (1%) 72 69	29, 42, 68, 111	0
1	B	189/196 (96%)	0.06	2 (1%) 80 80	27, 44, 67, 96	0
1	C	190/196 (96%)	0.06	2 (1%) 80 80	28, 45, 68, 88	0
1	D	189/196 (96%)	0.10	3 (1%) 72 69	23, 42, 67, 98	0
2	W	20/20 (100%)	0.39	1 (5%) 28 26	37, 57, 93, 102	0
2	Z	20/20 (100%)	0.15	0 100 100	33, 58, 100, 115	0
All	All	793/824 (96%)	0.07	11 (1%) 75 74	23, 44, 71, 115	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	ILE	5.1
1	C	7	ILE	4.4
2	W	1	DT	3.9
1	D	48	ARG	3.5
1	D	8	ASN	2.8
1	A	9	ARG	2.5
1	B	48	ARG	2.3
1	D	39	VAL	2.2
1	A	149	PHE	2.1
1	C	151	VAL	2.0
1	B	40	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.